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Rational Approximation and Remote Temperature Sensing

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In recent years there have been a number of papers dealing with methods for remote temperature sensing based on applying transform theory to the radiative transfer equation. In particular, methods based on optical measure theory method have the advantage that they do not require computations of numerical derivatives. In this paper we present techniques for approximating the radiance profile based on rational interpolation and nonlinear least squares data fitting. Optical measure theory permits the inversion of non-Laplacian exponential kernels. The models developed are easily extended to include generalized exponential weighting functions. We also introduce the concept of total nonlinear least squares data fitting.

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RATIONAL APPROXIMATION AND REMOTE TEMPERATURE SENSING

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1 INTRODUCTION

In recent years there have been a number of papers dealing with methods for remote temperature sensing based on applying transform theory to the radiative tranfer equation. King, Hohlfeld, and Kilian (1989) have shown that using differential inversion it is possible to successfully determine temperature profiles from measurements of the upwelling intensities in the atmosphere. In this research project an alternative transform method based on optical measure theory is developed. Previous work on this method has been carried out by by King and Leon (1989,1990) and by Leon (1990). The optical measure theory method has the advantage that it does not require any computations of numerical derivatives. Instead the radiance profile is approximated by a rational function. The Planck intensity is then determined as the inverse transform of the rational function.

In Section 2 we present techniques for approximating the radiance profile based on rational interpolation and nonlinear least squares data fitting. Optical measure theory permits the inversion of non-Laplacian exponential kernels. Consequently, in Section 3, we extend the mathematical models to include generalized exponential weighting functions. In Section 4 we discuss alternative nonlinear data fitting techniques. In particular we introduce the

concept of total nonlinear least squares data fitting. Some test results are presented in Section 5 and conclusions follow in Section 6.

2 RATIONAL APPROXIMATION OF RADIANCE PROFILES

Using radiative transfer theory one can relate the Planck intensity to the upwelling intensity of the atmosphere. This relationship can be expressed in terms of an integral equation of the first kind. Specifically the relationship is given by

$$R(\hat{p}) = \int_0^\infty B(p)\mathcal{W}(p/\hat{p})dp/p \tag{1}$$

where $\mathcal{W}(p/\hat{p})$ is a kernel weight function that peaks at $p = \hat{p}$ and $R(\hat{p})$ denotes the radiance of the wavelength channel whose weight function peaks at $p = \hat{p}$.

If we set

$$\mathcal{W}(z) = ze^{-z} \quad \text{and} \quad s = \frac{1}{\hat{p}}$$

then equation (1) can be expressed as a Laplace transform and consequently we can solve for the Planck function

$$B(p) = \mathcal{L}^{-1}\left(\frac{R(\frac{1}{s})}{s}\right)$$

We can think of $B(p)$ and $R(\hat{p})$ as transform pairs. Once a representation for R has been decided upon, then B can be determined analytically as an inverse Laplace transform.

The H-function inversion theory of Chandrasekhar, (1950) suggests that R should be represented as a rational function. If we set

$$R(\hat{p}) = d_1 + d_2\hat{p} + \cdots + d_{j+1}\hat{p}^j + \sum_{i=1}^{l} \frac{w_i}{1 + c_i\hat{p}} \tag{2}$$

then

$$\frac{R(\frac{1}{s})}{s} = \frac{d_1}{s} + \frac{d_2}{s^2} + \cdots + \frac{d_{j+1}}{s^j} + \sum_{i=1}^{l} \frac{w_i}{s + c_i}$$

and

$$B(p) = d_1 + d_2p + \cdots + \frac{d_{j+1}}{j!}p^j + \sum_{i=1}^{l} w_ie^{-c_ip} \tag{3}$$

The coefficients in equation (2) can be determined from the data by rational interpolation or by nonlinear least squares. Denote the radiance value corresponding to $\hat{p}_i$ by R_i for $i = 1,\ldots,m$ If one represents the radiance function as a rational function of the form

$$R(\hat{p}) = \frac{a_1\hat{p}^n + a_2\hat{p}^{n-1} + \cdots + a_{n+1}}{\hat{p}^l - a_{n+2}\hat{p}^{l-1} - \cdots - a_m} \qquad (n + l = m - 1)$$

then R will interpolate $(\hat{p}_i, R_i)$ if and only if

$$a_1\hat{p}_i{}^n + a_2\hat{p}_i{}^{n-1} + \cdots + a_{n+1} + a_{n+2}\hat{p}_i{}^{l-1}R_i + \cdots + a_m R_i = \hat{p}_i{}^l R_i \qquad (4)$$

$i = 1,\ldots,m$

The coefficients a_i are determined by solving the linear system (4). The residue form of R can be computed as an inverse convolution and from this one can determine the coefficients for equations (2) and (3). Generally these equations need only have a small number of components. It is possible to get a good fit with $j = 1,2$ or 3 and $l = 1$ or 2. If one takes $j = 2$ and $l = 2$, it is possible that for some data sets the interpolating function will have a positive pole, $(c_i < 0)$, even though this is impossible for an actual radiance profile. When this happens the weight w_i corresponding to the pole will be much smaller than the weight corresponding to the other rational component. Thus if one sets $w_i = 0$, then the resulting function will give a good approximation to the data points.

In practice one can obtain a better approximation to the radiance data and avoid the problem of positive poles by using nonlinear least squares. The rational interpolating function can be taken as starting approximation for an iteratively computed nonlinear least squares fit to the data of the form

$$R(\hat{p}) = x_1 + x_2\hat{p} + \cdots + x_{j+1}\hat{p}^j + \sum_{i=1}^{l} \frac{x_{j+1+i}}{1 + x_{j+1+l+i}^2\hat{p}} \qquad (5)$$

Initially the x_i coefficients are determined from the coefficients of the rational interpolating function of the form (2). Whenever the interpolating function has a positive pole, i.e, a coefficient $c_i < 0$, one sets the corresponding coefficient $x_{j+1+l+i}$ in (5) equal to 1 and the weight x_{j+1+i} can be set equal to 0.

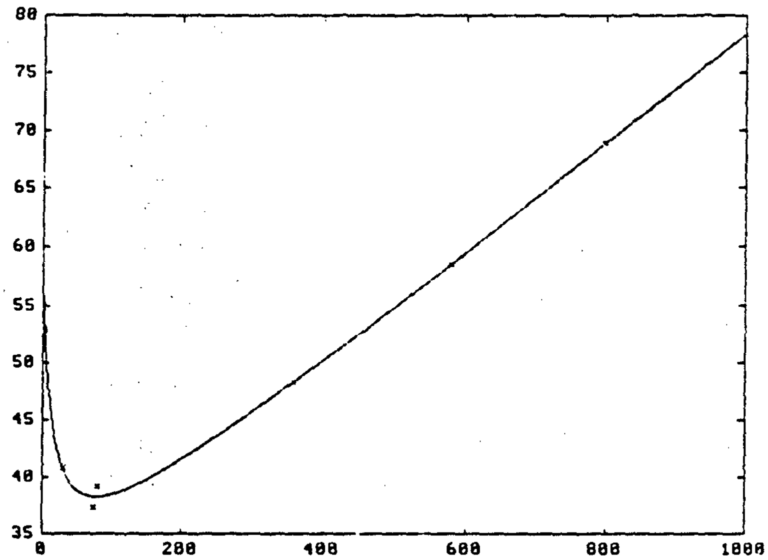

Figure 1. Nonlinear least squares radiance function for set of TOVS data

The choice of a rational function to represent the radiance data is motivated by the physics of the atmosphere. In practice the nonlinear least squares approximation gives a very good fit to the radiance data. The coefficients of the rational function can be used to determine a Planck function of the form (3).

In Figure 1, a least squares fit of the form (5) is given for a typical data set obtained from the NOAA TIROS Operational Vertical Sounder (TOVS).

3 GENERALIZED EXPONENTIAL INVERSION

We can obtain a natural generalization of our previous results by taking a more general form for the weight function. If we set

$$W(z) = W_k(z) = \gamma_k z \exp_k(z)$$

where

$$\gamma_k = \frac{1}{k^{1/k}\Gamma\left(\frac{k+1}{k}\right)}$$

and

$$\exp_k(z) = \exp(-z^k/k)$$

then it follows that

$$R(\hat{p}) = \int_0^\infty B(p)W_k(p/\hat{p})\frac{dp}{p}$$

If $R(\hat{p})$ is of the form (2), then the Planck intensity $B(p) = B_k(p)$ will be of the form

$$B_k(p) = d_1 + d_2 p + \cdots + \frac{d_{j+1}}{j!}p^j + \sum_{i=1}^{l} w_i \exp_k(c_i p) \tag{6}$$

Note that equations (3) and (6) are the same in the case $k = 1$.

4 TOTAL NONLINEAR LEAST SQUARES

A number of algorithms have been developed for nonlinear least squares fitting. Two algorithms using gradient methods to minimize the residual functions were developed specifically for rational fits of the form (5). These algorithms require good starting approximations and may converge to a local rather than a global minimum. The standard Nelder-Meade Simplex Algorithm, however, does seem to give satisfactory results even though convergence is rather slow. It may be possible to speed up convergence by taking some sort combination of the Nelder-Meade and gradient methods.

It should be noted that the standard nonlinear least squares techniques all seek to minimize the residual errors for the dependent variable. For the type of radiance fitting problem considered here, the values of the independent variable $\hat{p}$ are also determined from satellite data and may involve some error. In fact, early experiments seem to indicate that the computed Planck function is more sensitive to perturbations in the $\hat{p}_i$ values than to changes in the R_i values. In order to reflect this in the data fitting, algorithms have been devised for total nonlinear least squares fits. In this process the residual is defined in terms of the sum of the squares of the distances of the points $(\hat{p}_i,\ R_i)$ to tangent lines to the curve (5) at the points $(\hat{p}_i,\ R(\hat{p}_i))$. Indeed a parameter t has been incorporated into the data fitting algorithms to specify

which type of fit is used. If $t = 0$, then the usual nonlinear least squares fit is used to minimize the residuals of the dependent variable. If $t = 1$, then a total least squares fit is computed. If $t = 2$, then a rational least squares fit is computed to minimize the residuals of the independent variable. For values of t between 0 and 2, intermediate types of fits are computed.

5 TEST RESULTS

Equation (1) is an integral equation of the first kind and consequently the problem of finding a solution is ill-posed. In addition to testing the optical measure theory method we also tested some of the standard methods used for solving integral integral equations of the first kind.

The standard techniques involve discretizing the equation and adding regularization conditions. The problem is then translated into a linear system of equations with quadratic constraints. The constrained problem can be solved using the methods proposed by Gander, (1981). However, when these techniques were applied to data sets obtained from the NOAA TIROS Operational Vertical Sounder (TOVS), the resulting matrices had very low numerical rank. Consequently, even with regularization conditions we were unable to obtain meaningful results. On the other hand, the transform methods have smoothness constraints and additional structure built in. The rational form (2) can be computed in a numerically stable manner and the coefficients define a unique Planck function.

The interpolation and nonlinear least squares algorithms have been tested extensively on simulated data and on the TOVS data. The algorithms are numerically stable. Figures 2 through 5 represent Planck functions that were generated using the same data set as in Figure 1. Figure 2 shows a semilog plot of the Planck function. The pressures are given in millibars on the vertical axis. Figure 3 shows the Planck function for the data set derived by generalized exponential inversion with $k = 0.8$. Figure 4 shows the Planck function derived by generalized exponential inversion with $k = 1.2$. Figure 5 shows all three Planck functions plotted as functions of p on the same axis system.

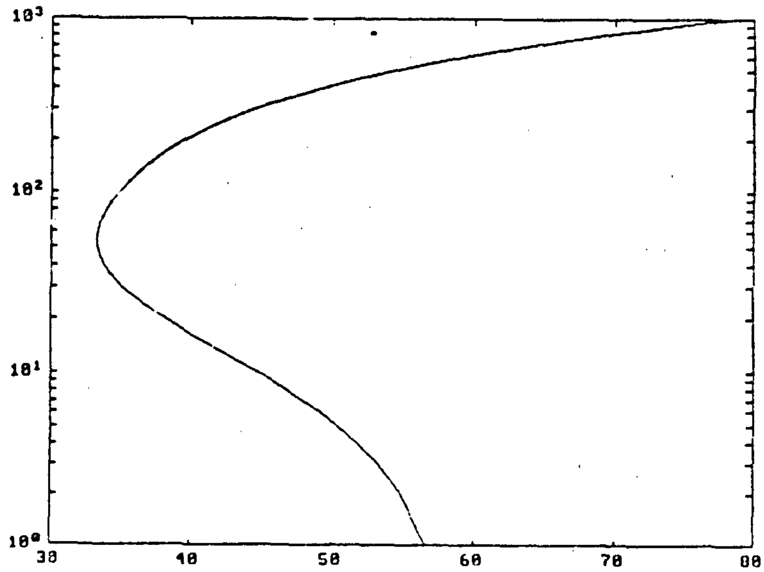

Figure 2. Planck intensity derived from set of TOVS data

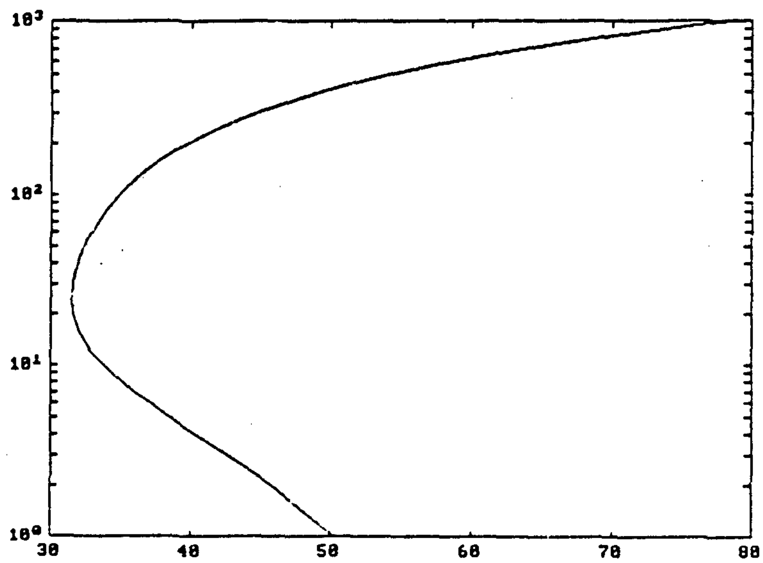

Figure 3. Generalized exponential inversion with $k = 0.8$

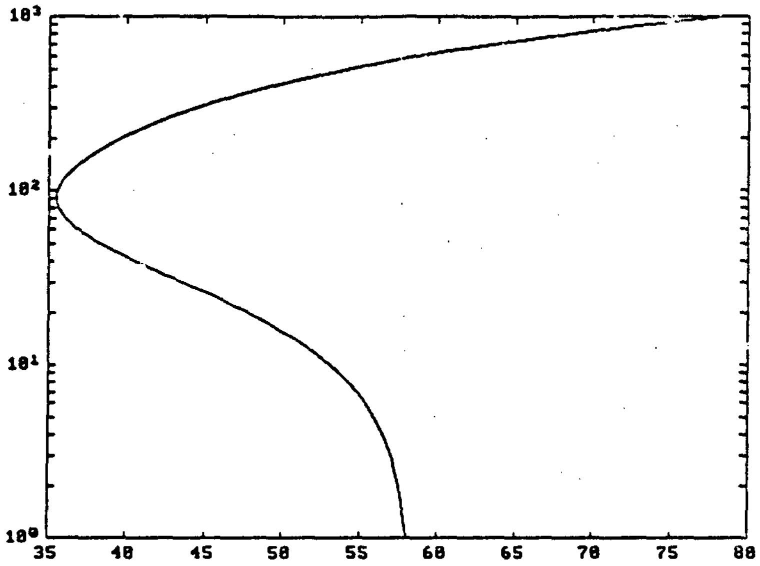

Figure 4. Generalized exponential inversion with $k = 1.2$

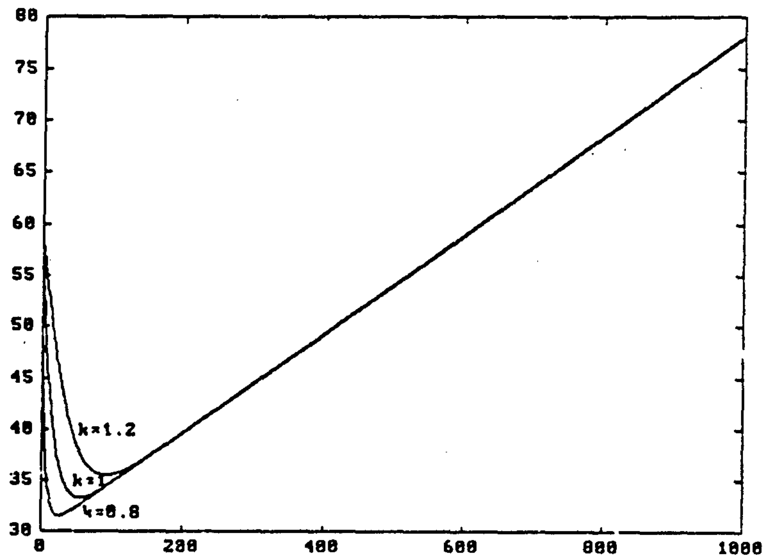

Figure 5. $k = 0.8,\ 1,\ 1.2$ inverses

The question that still is outstanding is how to choose j, the degree of the polynomial component of the fit, and how to choose l, the number of hyperbolic components. Although it is reasonable that both of these numbers should be relatively small, it is not possible to give a definitive answer as to the optimal values of j and l based solely on the TOVS data sets and simulated data. It is anticipated that these questions will be answered when future data sets with more sensing channels in the appropriate ranges become available.

6 CONCLUSIONS

Although transfer theory can be used to relate the Planck intensity to the upwelling intensity in the atmosphere, the relation is expressed in the form of an integral equation of the first kind. Such equations are ill-posed and consequently do not have unique numerical solutions. Adding regularization conditions does not solve the problem. For data sets like those obtained from the TOVS data, there is not enough information to determine the Planck function using matrix methods with appropriate smoothness constraints. More assumptions relative to the physics of the atmosphere must be added. In this regard the transform methods based on optical measure theory seem to work well. The key step is the representation of the radiance profile by a rational function. This can be accomplished in a numerically stable manner using nonlinear least squares fitting algorithmns.

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